

=> d his

(FILE 'HOME' ENTERED AT 11:50:04 ON 19 AUG 2004)

L1 FILE 'CAPLUS' ENTERED AT 11:50:15 ON 19 AUG 2004  
STRUCTURE UPLOADED  
S L1

L2 FILE 'REGISTRY' ENTERED AT 11:50:44 ON 19 AUG 2004  
13 S L1

L3 FILE 'CAPLUS' ENTERED AT 11:50:45 ON 19 AUG 2004  
12 S L2

FILE 'STNGUIDE' ENTERED AT 11:52:47 ON 19 AUG 2004

FILE 'CAPLUS' ENTERED AT 11:55:21 ON 19 AUG 2004

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	63.14
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-8.82

FILE 'CAPLUS' ENTERED AT 11:55:38 ON 19 AUG 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 19 Aug 2004 VOL 141 ISS 8  
FILE LAST UPDATED: 18 Aug 2004 (20040818/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1 full

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 11:55:50 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 27503 TO ITERATE

100.0% PROCESSED 27503 ITERATIONS 543 ANSWERS  
SEARCH TIME: 00.00.01

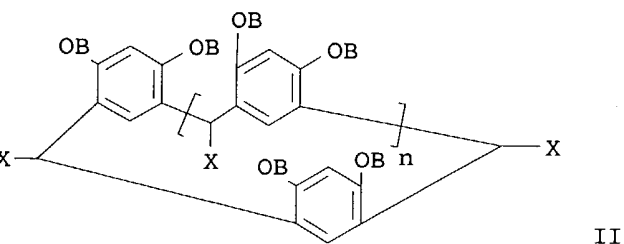
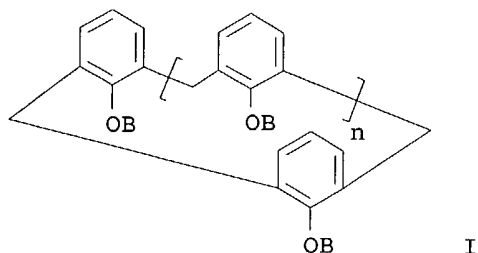
L4 543 SEA SSS FUL L1

L5 134 L4  
=> s 15 and (halo? fluor?)  
354051 HALO?  
1023157 FLUOR?  
1332 HALO? FLUOR?  
(HALO? (W) FLUOR?)  
L6 0 L5 AND (HALO? FLUOR?)  
=> s 15 and (halogen)  
100468 HALOGEN  
L7 4 L5 AND (HALOGEN)  
=> d 1-4 ibib abs hitstr

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:870678 CAPLUS  
DOCUMENT NUMBER: 139:371613  
TITLE: Light-emitting compositions containing calixarenes or calixresorcinarenes suitable for preparation of electroluminescent devices  
INVENTOR(S): Takahashi, Naoto; Hyakuta, Junji; Kawabata, Yuichiro  
PATENT ASSIGNEE(S): Tokuyama Corp., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 38 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003313546	A2	20031106	JP 2002-122730	20020424
PRIORITY APPLN. INFO.:			JP 2002-122730	20020424
OTHER SOURCE(S):		MARPAT 139:371613		

GI



AB The compns. contain 0.1-90 weight% calixarenes or calixresorcinarenes having light-emitting organic groups or charge-transferring organic groups and 10-99.9 weight% vinylcarbazole. The preferable structures for calixarenes or calixresorcinarenes are A substituted on each benzene ring of I or II (A,

. B, X = H, **halogen**, alkyl, aryl, alkoxy with  $\geq 1$  of A, B,  
and X being YmZ; Y = bivalent organic group; Z = light-emitting organic group,  
charge-transferring organic group; m = 0, 1; n = integer of 1-18).

546632-74-0P

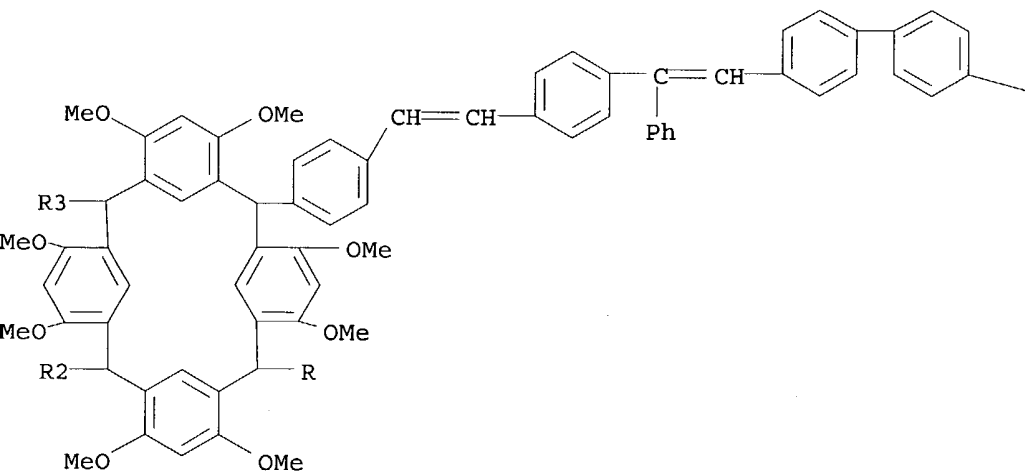
RL: IMF (Industrial manufacture); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)

(light-emitting calixarene or calixresorcinarene compns. for  
electroluminescent devices)

546632-74-0 CAPLUS

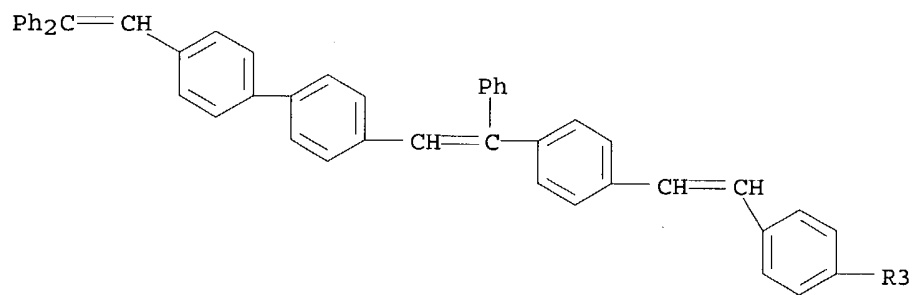
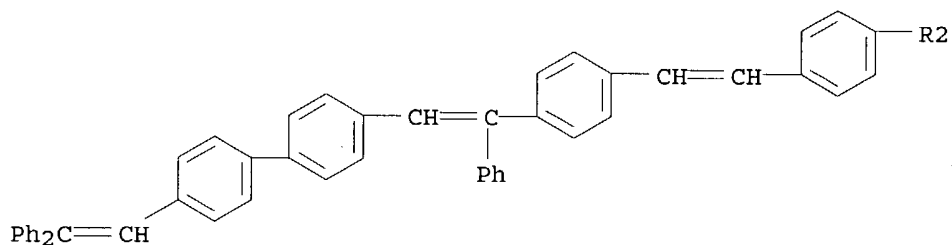
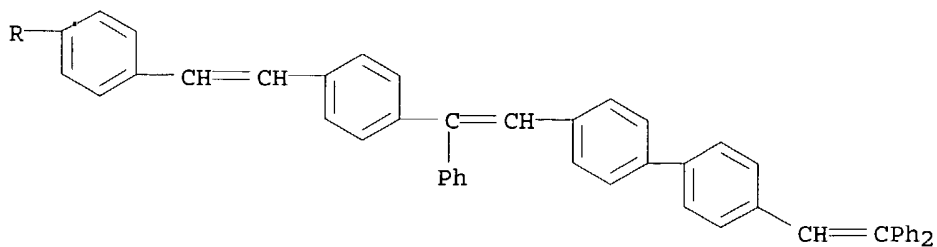
Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),1  
5,17,19(26),21,23-dodecaene, 2,8,14,20-tetrakis[4-[2-[4-[2-[4'-(2,2-  
diphenylethenyl)[1,1'-biphenyl]-4-yl]-1-phenylethenyl]phenyl]ethenyl]phenyl  
1]-4,6,10,12,16,18,22,24-octamethoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

CH=CPh<sub>2</sub>



546631-70-3 546632-68-2 546632-71-7

RL: RCT (Reactant); RACT (Reactant or reagent)

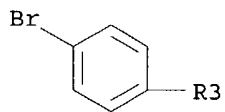
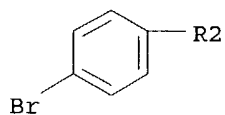
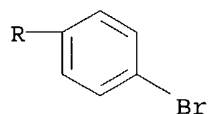
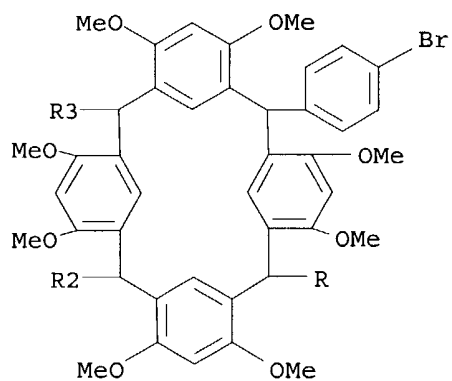
(light-emitting calixarene or calixresorcinarene compns. for electroluminescent devices)

546631-70-3 CAPLUS

Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),1

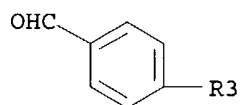
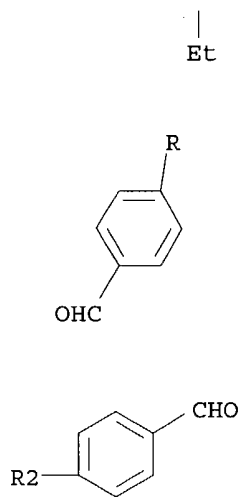
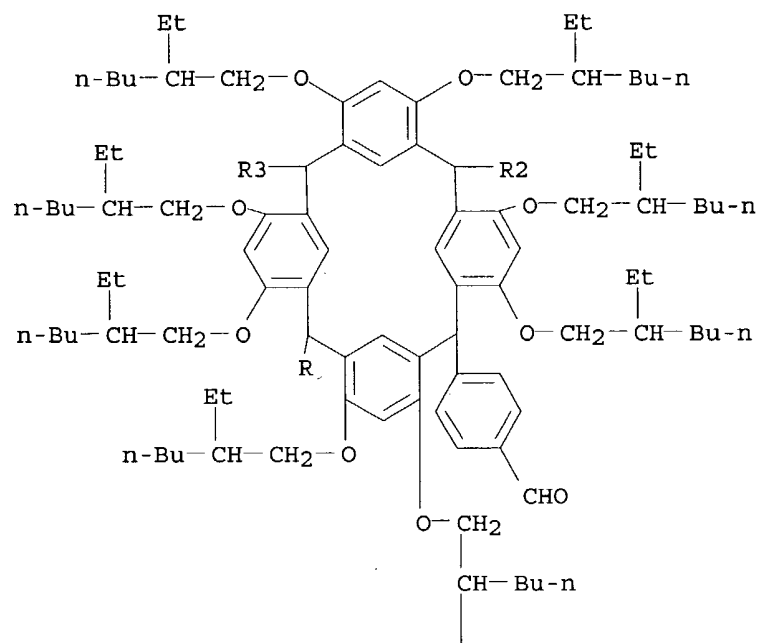
5,17,19(26),21,23-dodecaene, 2,8,14,20-tetrakis(4-bromophenyl)-

4,6,10,12,16,18,22,24-octamethoxy- (9CI) (CA INDEX NAME)



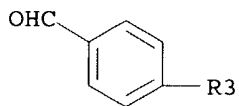
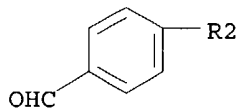
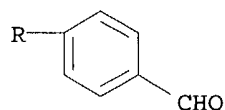
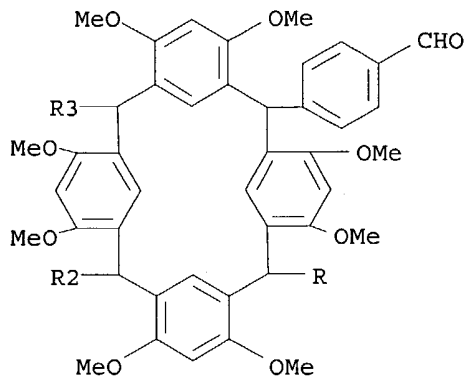
546632-68-2 CAPLUS

Benzaldehyde, 4,4',4'',4'''-[4,6,10,12,16,18,22,24-octakis[(2-ethylhexyl)oxy]pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-2,8,14,20-tetrayl]tetrakis- (9CI) (CA INDEX NAME)



546632-71-7 CAPLUS

Benzaldehyde, 4,4',4'',4'''-(4,6,10,12,16,18,22,24-octamethoxypentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-2,8,14,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)



ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN  
 CESSION NUMBER: 2003:300651 CAPLUS  
 CUMENT NUMBER: 138:326558  
 TLE: Preparation of hexameric calixarene-type complexes and  
 their use for encapsulation of pharmaceutically active  
 agents  
 VENTOR(S): Atwood, Jerry L.  
 TENT ASSIGNEE(S): USA  
 URCE: U.S. Pat. Appl. Publ., 14 pp.  
 CODEN: USXXCO  
 CUMENT TYPE: Patent  
 NGUAGE: English  
 MILY ACC. NUM. COUNT: 1  
 TENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073872	A1	20030417	US 2001-978925	20011016
WO 2003033649	A2	20030424	WO 2002-US30460	20020925
WO 2003033649	A3	20030703		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,

CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
NE, SN, TD, TG

PRIORITY APPLN. INFO.:

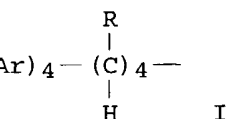
US 2001-978925

A 20011016

OTHER SOURCE(S):

MARPAT 138:326558

I



The invention relates to a composition I [wherein Ar = trihydroxybenzene radical; R = (alkyl)aryl group containing 6-20 C atoms, an aliphatic group containing 2-20 C atoms, or a substituted aliphatic or (alkyl)aryl group having a substituent of carbonyl, carboxyl, amide, halide, ester, or hydroxyl group], comprising a highly stable guest/host assembly having a spheroidal host assembly comprised of a hexamer of a methylene-bridged trihydroxybenzene tetramer and a guest component encapsulated within the spheroidal host assembly. The invention also relates to a guest component, specifically a pharmaceutically active agent, that is encapsulated within the spheroidal host assembly and is stable upon a solubilization in a 1:1 mixture of acetone and H<sub>2</sub>O for one day at 37°. The pharmaceutically active agent encapsulated within the spheroidal hexamer may be Depakote, Wellbutrin, Allegra, Neurontin, Zovirax, or Claritin. Another aspect of the invention provides for a process for the preparation of a hexameric complex from a methylene-bridged tetramer solubilized in an amphiphilic organic solvent. An activator, comprising an organic compound of a lower mol. weight than that of the tetramer which is functionalized with at least one of an acidic group, **halogen**, amino group, amido group, ester group, or hydroxy group, is incorporated into the amphiphilic solvent containing the tetramer. The tetramer may be prepared from an aldehyde and pyrogallol which are reacted under conditions to produce a condensation product of the methylene-bridged cyclic tetramer. For example, stepwise addition of concentrated HCl and propionaldehyde to a solution of pyrogallol in 95% EtOH, followed by stirring for 12 h afforded I (R = Et).

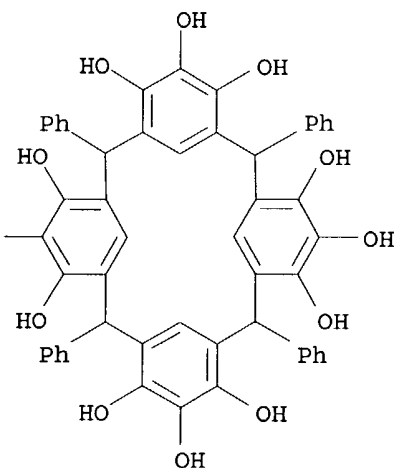
512785-41-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(hexameric capsule; preparation of hexameric calixarene-type complexes and their use for encapsulation of pharmaceutically active agents)

512785-41-0 CAPLUS

Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,5,6,10,11,12,16,17,18,22,23,24-dodecol, 2,8,14,20-tetraphenyl- (9CI) (CA INDEX NAME)





ACCESSION NUMBER: 1995:828347 CAPLUS  
 DOCUMENT NUMBER: 123:241910  
 TITLE: Friction charge-providing member for positively-chargeable toner.  
 INVENTOR(S): Mukudai, Osamu; Matsuura, Yuuji; Niimura, Isao; Watanabe, Kayoko; Iwasa, Keiko  
 PATENT ASSIGNEE(S): Hodogaya Chemical Co., Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 22 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 655658	A2	19950531	EP 1994-105509	19940408
EP 655658	A3	19960703		
R: DE, FR, GB				
JP 07128916	A2	19950519	JP 1993-293798	19931101
JP 08262871	A2	19961011	JP 1994-93926	19940408
PRIORITY APPLN. INFO.:			JP 1993-293798	19931101

OTHER SOURCE(S): MARPAT 123:241910

I For diagram(s), see printed CA Issue.

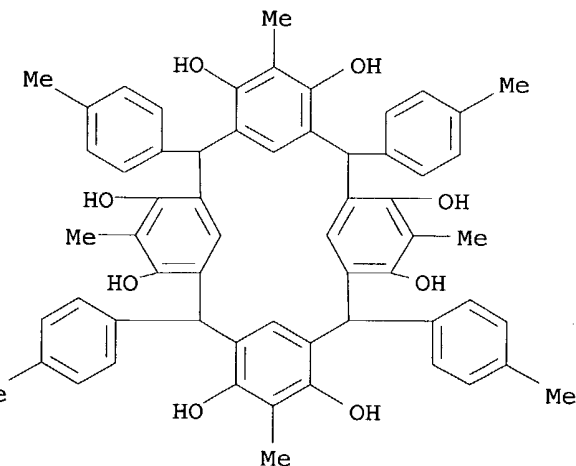
B A friction charge-providing member for pos.-chargeable toner comprises a parent material and a charge-controlling agent on the surface selected from I and II [A and B = H, **halogen**, alkoxyl, carboxyl, hydroxyl, ester, nitro, amino, alkylamino, alkyl which may contain a substituent(s) or a Ph group which may contain a substituent(s); R = H, alkyl or Ph or naphthyl group which may contain a substituent(s); m = an integer 2 to 16; and n = an integer 4 to 8]. The toner provides improved charging stability.

T **168405-65-0**

RL: TEM (Technical or engineered material use); USES (Uses)  
 (charge-controlling agent for electrostatog. toner)

N 168405-65-0 CAPLUS

N Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol, 5,11,17,23-tetramethyl-2,8,14,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1995:794919 CAPLUS  
 DOCUMENT NUMBER: 123:325712  
 TITLE: Electrostatic image developing toner.  
 INVENTOR(S): Mukudai, Osamu; Matsuura, Yuuji; Niimura, Isao;

PATENT ASSIGNEE(S): Watanabe, Kayoko; Isawa, Keito  
 SOURCE: Hodogaya Chemical Co., Ltd., Japan  
 Eur. Pat. Appl., 22 pp  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 651294	A1	19950503	EP 1994-105508	19940408
EP 651294	B1	19980708		
R: DE, FR, GB				
JP 07175269	A2	19950714	JP 1994-93927	19940408
US 5679489	A	19971021	US 1996-620150	19960322
PRIORITY APPLN. INFO.:			JP 1993-293799	19931101
			US 1994-224523	19940407

OTHER SOURCE(S): MARPAT 123:325712

GI For diagram(s), see printed CA Issue.

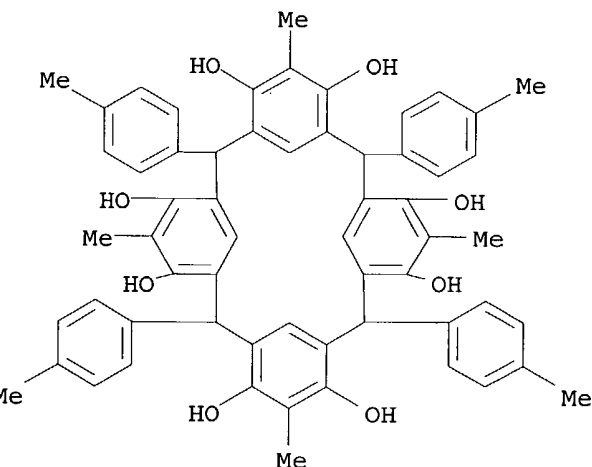
AB An electrophotog. toner free of metal such as Cr comprises  $\geq 1$   
 charge-controlling agent selected from I and II [A, B = H, **halogen**  
 , alkoxy carboxyl, OH, ester, nitro, amino, alkylamino, alkyl, Ph; R = H,  
 alkyl, Ph, naphthyl; m = 2-16; n = 4-8]. The toner shows no deterioration  
 during preparation, excellent stability, excellent dispersibility in binder  
 resin, and excellent friction chargeability.

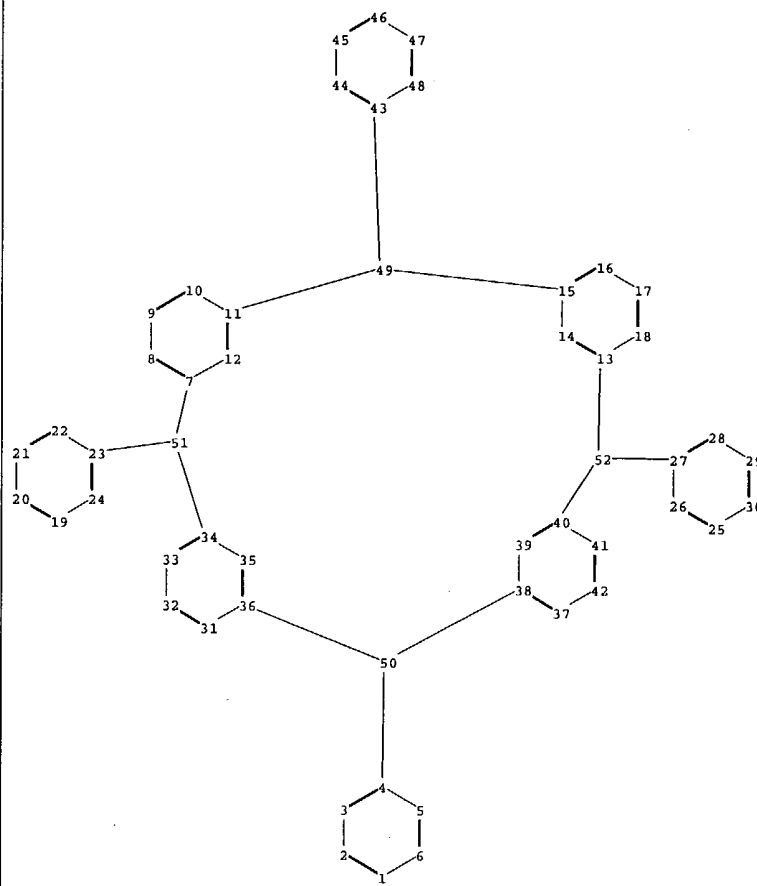
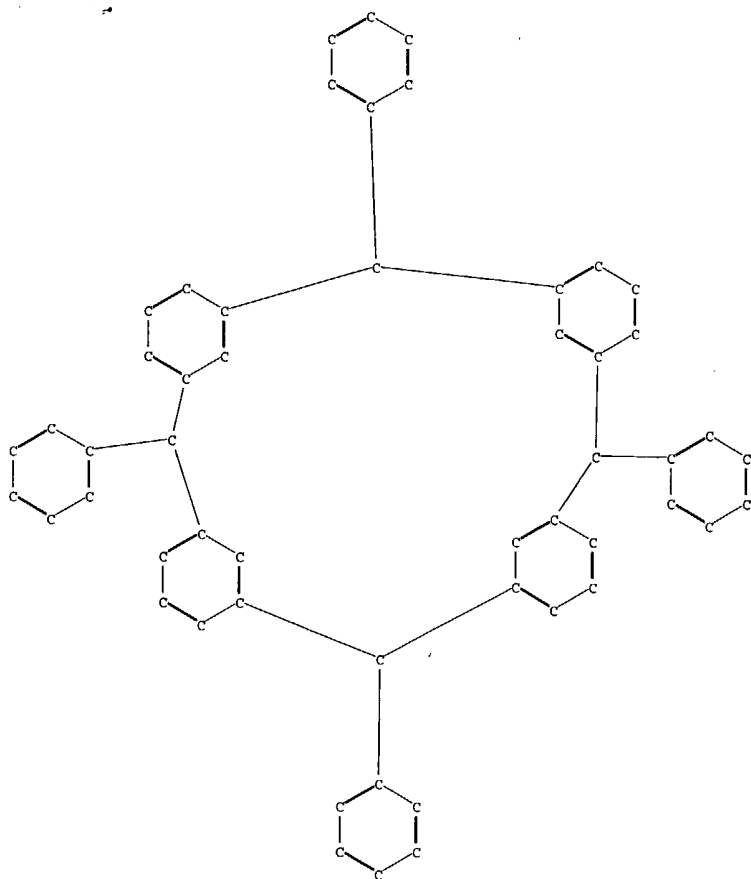
IT 168405-65-0

RL: MOA (Modifier or additive use); USES (Uses)  
 (charge-controlling agent for electrophotog. toners)

RN 168405-65-0 CAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),1  
 5,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol,  
 5,11,17,23-tetramethyl-2,8,14,20-tetrakis(4-methylphenyl)- (9CI) (CA  
 INDEX NAME)





ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25  
 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48  
 49 50 51 52

chain bonds :

4-50 23-51 27-52 43-49

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-51 8-9 9-10 10-11 11-12 11-49 13-14 13-18  
 13-52 14-15 15-16 15-49 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 25-26  
 25-30 26-27 27-28 28-29 29-30 31-32 31-36 32-33 33-34 34-35 34-51 35-36 36-50  
 37-38 37-42 38-39 38-50 39-40 40-41 40-52 41-42 43-44 43-48 44-45 45-46 46-47  
 47-48

exact/norm bonds :

7-51 11-49 13-52 15-49 34-51 36-50 38-50 40-52

exact bonds :

4-50 23-51 27-52 43-49

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15  
 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 25-26 25-30 26-27 27-28  
 28-29 29-30 31-32 31-36 32-33 33-34 34-35 35-36 37-38 37-42 38-39 39-40 40-41  
 41-42 43-44 43-48 44-45 45-46 46-47 47-48

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom  
 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom  
 52:Atom

SAMPLE SEARCH INITIATED 11:50:44 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1336 TO ITERATE

74.9% PROCESSED 1000 ITERATIONS 13 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 24528 TO 28912  
PROJECTED ANSWERS: 97 TO 597

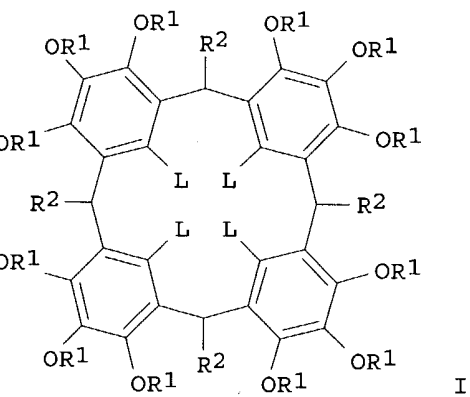
L2 13 SEA SSS SAM L1

L3 12 L2

=> d 1-12 ibib abs hitstr

L3 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:947709 CAPLUS  
DOCUMENT NUMBER: 140:16573  
TITLE: Preparation of calixarene-derivatives having  
anti-viral activity  
INVENTOR(S): Coveney, Donal; Costello, Benjamin  
PATENT ASSIGNEE(S): Aids Care Pharma, Limited, Ire.  
SOURCE: Eur. Pat. Appl., 22 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1367044	A1	20031203	EP 2003-76538	20030521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			EP 2003-76538	20030521
OTHER SOURCE(S): CASREACT 140:16573; MARPAT 140:16573				
GI				



AB The patent relates to the preparation of compds. I wherein at least one R1 = H and the remainder = CH2CO2K; R2 = 4-fluorophenyl; and L = H. The compds.

are useful as pharmaceutical compns. in the treatment of AIDS. Thus, a pyrogallol calixarene derivative prepared by reacting pyrogallol and p-fluorobenzaldehyde to form pyrogallol calixarene; treated with potassium carbonate and Et bromoacetate; and followed by hydrolysis gave EC50 of 1.25  $\mu$ M compared to 0.5-1.0 for the control (AC-1) in HIV-1 antiviral assay.

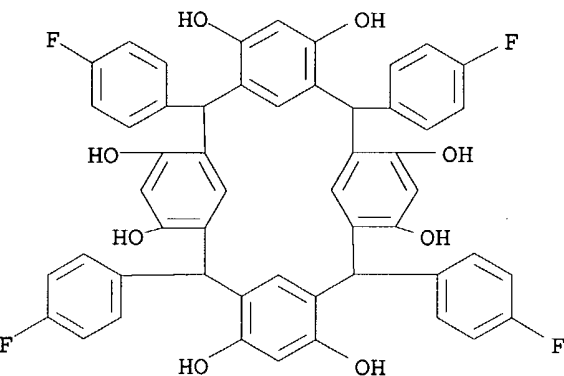
IT 629614-96-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of calixarene-derivs. having anti-viral activity)

RN 629614-96-6 CAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol, 2,8,14,20-tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:913398 CAPLUS

DOCUMENT NUMBER: 137:278960

TITLE:

Solvent-free synthesis of calix[4]resorcinarenes

AUTHOR(S):

Roberts, Brett A.; Cave, Gareth W. V.; Raston, Colin L.; Scott, Janet L.

CORPORATE SOURCE:

Centre for Green Chemistry, Monash University, 3800, Australia

SOURCE:

Green Chemistry (2001), 3(6), 280-284

CODEN: GRCHFJ; ISSN: 1463-9262

PUBLISHER:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 137:278960

AB Calix[4]resorcinarenes may be prepared in high yield and purity by direct reaction of resorcinol and benzaldehyde derivs. in the presence of a catalytic amount of solid acid and at ambient temperature under solvent-free conditions. This represents a viable alternative to traditional solution phase methodol. The solvent-free method measures up well with respect to energy usage, solvent wastes and associated hazards, reaction time and yield. In addition, the relevant benzaldehyde derivs. are prepared in polypropylene glycol, which is readily recycled.

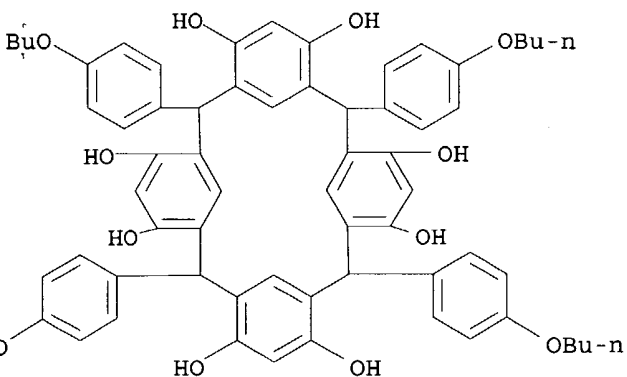
IT 464885-60-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and crystal structure of calix[4]resorcinarenes via cyclocondensation of arylaldehydes with resorcinol under solvent-free conditions)

RN 464885-60-7 CAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol, 2,8,14,20-tetrakis(4-butoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

SSION NUMBER: 2001:765663 CAPLUS

MENT NUMBER: 136:69555

E: A vibrational spectroscopic study of clathrates of resorcarene-based cavitands

OR(S): Dormann, Jorg; Ruoff, Andreas; Schatz, Jurgen; Middel, Oskar; Verboom, Willem; Reinhoudt, David N.

ORATE SOURCE: Section of Vibrational Spectroscopy, University of Ulm, Ulm, D-89069, Germany

CE: Journal of Physical Organic Chemistry (2001), 14(10), 704-708

CODEN: JPOCEE; ISSN: 0894-3230

ISHER: John Wiley & Sons Ltd.

MENT TYPE: Journal

JAGE: English

By comparison of the fully assigned vibrational spectra obtained for resorcarene-based cavitands, their clathrates with toluene and ethanol resp., and free guest mols., good structural models for the clathrates could be obtained merely based on Fourier transform IR data. Using this technique, various different interactions between the host and guest in the solid state as well as the orientation of the included guest could be identified. In the case of one cavitand, the model obtained by this methodol. could be validated by comparison with an exptl. crystal structure anal.

**384379-14-0**

RL: PRP (Properties)

(IR study on clathrates of resorcarene-based cavitands)

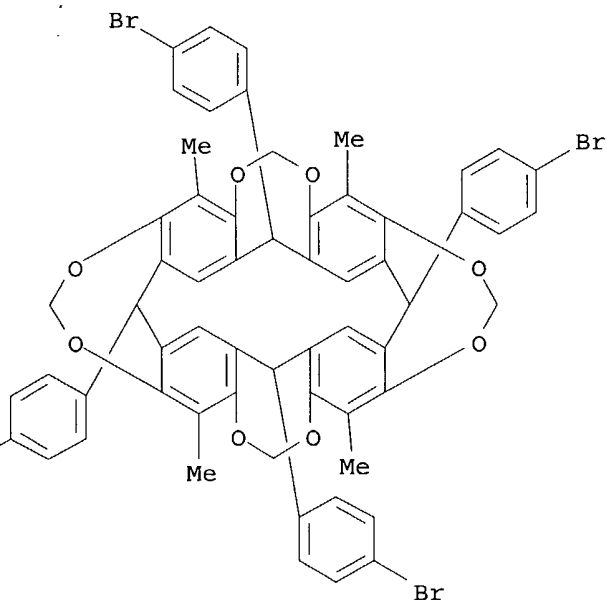
384379-14-0 CAPLUS

2,20:3,19-Dimetheno-1H,21H,23H,25H-bis[1,3]dioxocino[5,4-i:5',4'-i']benzo[1,2-d:5,4-d']bis[1,3]benzodioxocin, 1,21,23,25-tetrakis(4-bromophenyl)-7,11,15,28-tetramethyl-, stereoisomer, compd. with methylbenzene (1:4) (9CI) (CA INDEX NAME)

CM 1

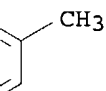
CRN 216760-27-9

CMF C60 H44 Br4 O8



CM 2

CRN 108-88-3  
CMF C7 H8



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN  
SESSION NUMBER: 2001:656593 CAPLUS  
DOCUMENT NUMBER: 135:371514  
TITLE: Novel resorcin[4]arenes as potassium-selective ion-channel and transporter mimics  
AUTHOR(S): Wright, Angela J.; Matthews, Susan E.; Fischer, Wolfgang B.; Beer, Paul D.  
INSTITUTE SOURCE: Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, OX1 3QR, UK  
JOURNAL SOURCE: Chemistry--A European Journal (2001), 7(16), 3474-3481  
CODEN: CEUJED; ISSN: 0947-6539  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal  
LANGUAGE: English

A series of novel resorcin[4]arenes with extended  $\pi$  systems have been synthesized and developed as potassium-selective transporters. Resorcin[4]arenes that feature crown ether moieties function as efficient carriers of  $K^+$  across bulk liquid membranes showing enhanced selectivity over the other alkali metal ions relative to a model system (benzo[15]crown-5). Incorporation of functionalities suitable for pore formation, in addition to an extra annulus of aromatic residues, gives mols. which have remarkable ion-channel-mimicking behavior in a biol. lipid bilayer with outstanding  $K^+/Na^+$  selectivity.

374106-11-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of resorcin[4]arenes and activity as potassium-selective ion-channel and transporter mimics)

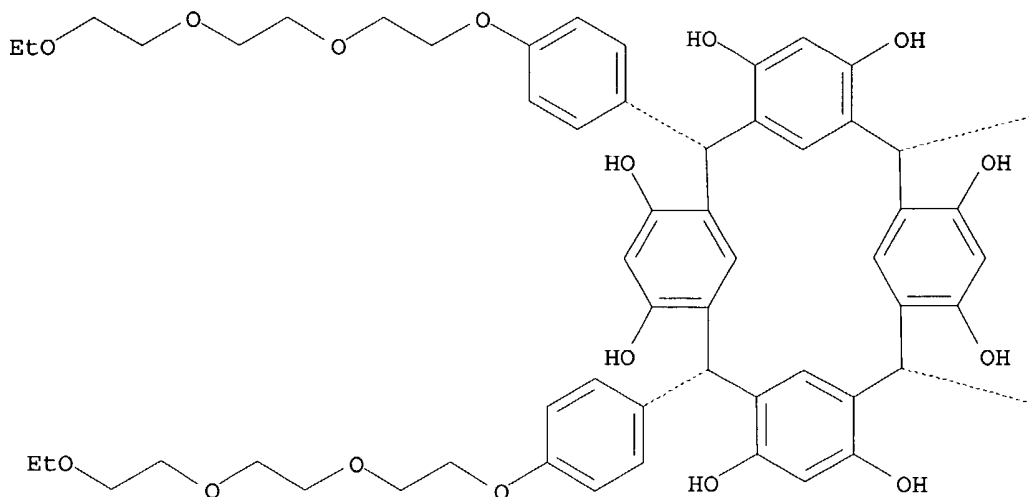
374106-11-3 CAPLUS

Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),1

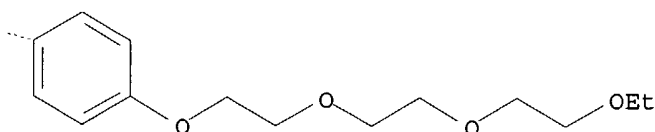
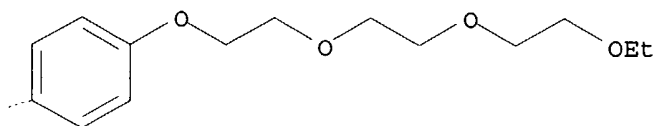
5,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol,  
2,8,14,20-tetrakis[4-[2-[2-(2-ethoxyethoxy)ethoxy]ethoxy]phenyl]-,  
stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:513131 CAPLUS  
DOCUMENT NUMBER: 131:293195  
TITLE: Novel dissolution inhibitors based on calixarene  
derivatives for use in chemical amplification resists  
AUTHOR(S): Ito, Hiroshi; Nakayama, Tomonari; Ueda, Mitsuru;  
Sherwood, Mark; Miller, Dolores  
CORPORATE SOURCE: IBM Almaden Research Center, San Jose, CA, 95120, USA  
SOURCE: Polymeric Materials Science and Engineering (1999),  
81, 51-52  
CODEN: PMSEDG; ISSN: 0743-0515  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English



AB

IT

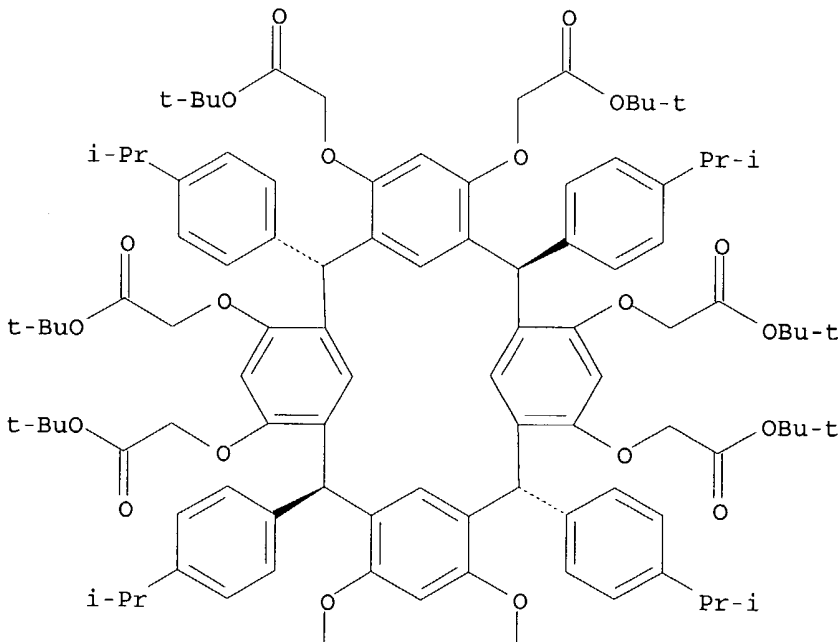
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

RN

CN

Re

PAGE 1-A



PAGE 2-A



REFERENCE COUNT:

L3 ANSWER 6 OF 12

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

AUTHOR (S) :

CORPORATE SOURCE: Institut de Recherches sur la Catalyse, Laboratoire de  
Catalyse et Synthèse Organique, Université Claude  
Bernard, Villeurbanne, 69622, Fr.

SOURCE: Journal of Inclusion Phenomena and Macrocyclic  
Chemistry (1999), 34(2), 141-151  
CODEN: JIPCF5

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

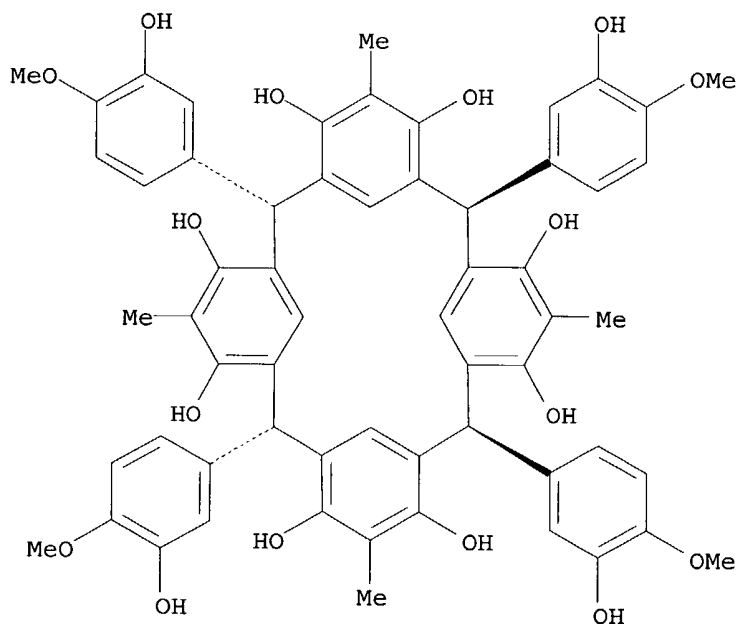
AB Combined nanofiltration-complexation is applied to the separation of Cs and Sr  
from a solution containing a large concentration of Na. Cs and Sr complexation was  
studied using various water soluble resorcinarene-type ligands. Combined  
with nanofiltration these ligands improved the separation of Cs and Sr from Na  
by the Filmtec NF 70 membrane.

IT 235094-96-9  
RL: NUU (Other use, unclassified); USES (Uses)  
(application of water soluble resorcinarenes in nanofiltration-  
complexation with cesium and strontium as targets)

RN 235094-96-9 CAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),1  
5,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol,  
2,8,14,20-tetrakis(3-hydroxy-4-methoxyphenyl)-5,11,17,23-tetramethyl-,  
stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:768661 CAPLUS

DOCUMENT NUMBER: 130:153434

TITLE: Rational Synthesis of Resorcarenes with Alternating  
Substituents at Their Bridging Methine Carbons

AUTHOR(S): Rumboldt, Giovanna; Boehmer, Volker; Botta, Bruno;  
Paulus, Erich F.

CORPORATE SOURCE: Dipartimento di Studi di Chimica e Tecnologia delle  
Sostanze Biologicamente Attive, Università La  
Sapienza, Rome, 00185, Italy

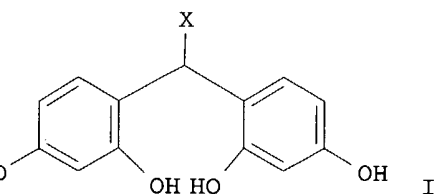
SOURCE: Journal of Organic Chemistry (1998), 63(26), 9618-9619  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:153434



Resorcarenes bearing different aldehyde residues in alternating order were prepared by condensation of resorcinol-derived dimers I (X = CH<sub>2</sub>CH<sub>2</sub>Ph, C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4) with 4-hydroxybenzaldehyde or propanal. Stereoisomers were obtained by chromatog. or by acetylation with subsequent chromatog.

**220213-30-9P**

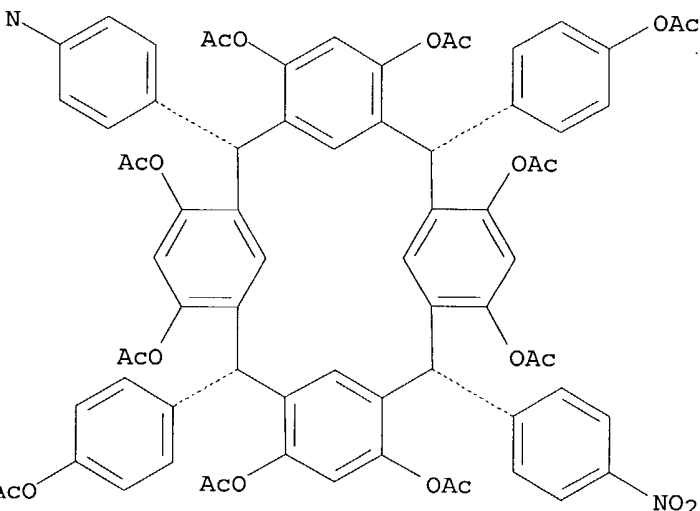
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of resorcarenes with alternating substituents at methine bridges)

220213-30-9 CAPLUS

Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octol, 2,14-bis[4-(acetyloxy)phenyl]-8,20-bis(4-nitrophenyl)-, octaacetate (ester), stereoisomer (9CI) (CA INDEX NAME)

relative stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

CESSION NUMBER: 1998:664722 CAPLUS

CUMENT NUMBER: 130:25128

TLE: Phosphacavitands: I. Phosphorylation of calix[4]resorcinolarenes with phosphorous amides. Synthesis of first cavitands derived from phosphoramidites

THOR(S): Maslennikova, V. I.; Shkarina, E. V.; Vasyanina, L. K.; Lysenko, K. A.; Antipin, M. Yu.; Nifant'ev, E. E.

RPORATE SOURCE: Moscow State Pedagogical University, Moscow, Russia  
URCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (1998), 68(3), 350-360

CODEN: RJGCEK; ISSN: 1070-3632

BLISHER: MAIK Nauka/Interperiodica Publishing

CUMENT TYPE: Journal

NGUAGE: English

Phosphorylation of calix[4]resorcinolarenes with phosphorous mono-, di-

and triamides was studied. Factors controlling the reaction pathways and the selectivity of the formation of cavitands with phosphite and phosphoramidite moieties and calix[4]resorcinolarenes with eight phosphite or phosphoramidite moieties were revealed.

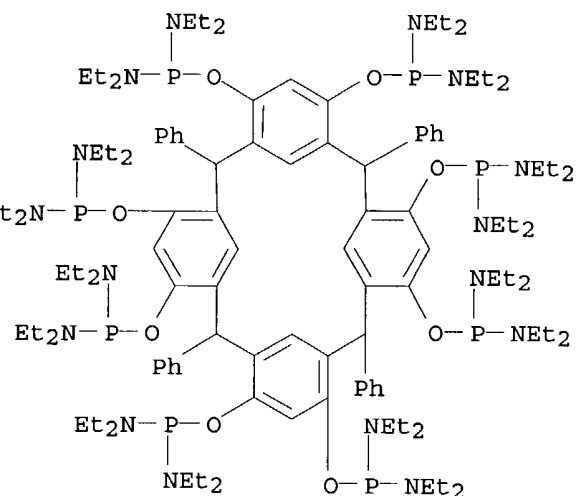
216078-73-8

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(preparation of cavitands derived from phosphoramidites)

216078-73-8 CAPLUS

Phosphorodiamidous acid, tetraethyl-, 2,8,14,20-tetraphenylpentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-4,6,10,12,16,18,22,24-octayl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

3 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:394118 CAPLUS

DOCUMENT NUMBER: 129:128942

TITLE: Toner for electrostatic latent image development

INVENTOR(S): Ueda, Hideaki; Furukawa, Keiichi

PATENT ASSIGNEE(S): Minolta Camera Co., Ltd., Peop. Rep. China

SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

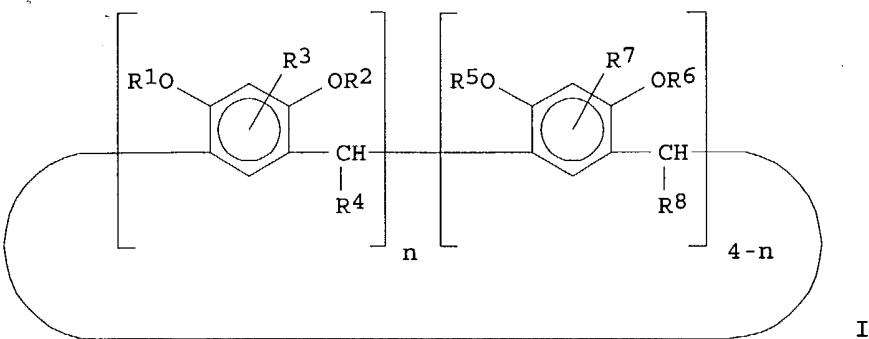
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10161349	A2	19980619	JP 1996-316063	19961127
PRIORITY APPLN. INFO.:			JP 1996-316063	19961127



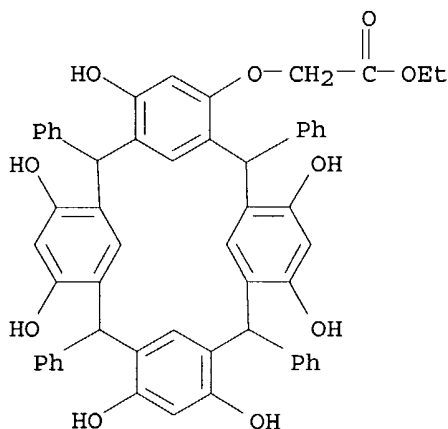
AB The title toner contains a resorcinol arene derivative I ( $R_1, R_2, R_5, R_6 = H$ , C1-5 alkyl,  $(CH_2)_mCO_2R_9$ ;  $R_9 = H$ , lower alkyl;  $m = 1-3$ ;  $R_1, R_2, R_5$ , and  $R_6$  cannot be H in the same time;  $R_3, R_7 = H$ , halo, alkoxy, carboxylnitro, alkyl, hydroxy;  $R_4, R_8 =$  alkyl, aryl, heterocyclyl;  $n = 1-4$ ) as a charge controlling agent. The toner shows superior charge stability, resistance to heat and solvent, color reproducibility and transparency.

IT 210303-17-6

RL: TEM (Technical or engineered material use); USES (Uses)  
(charge controlling agent for electrostatog. toner)

RN 210303-17-6 CAPLUS

CN Acetic acid, [(6,10,12,16,18,22,24-heptahydroxy-2,8,14,20-tetraphenylpentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaen-4-yl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:257156 CAPLUS

DOCUMENT NUMBER: 124:342828

TITLE: Designing of resorcinol-p-hydroxybenzaldehyde tetramer for uranophilic activity

AUTHOR(S): Singh, Harmit; Singh, Serjinder

CORPORATE SOURCE: Dep. Chem., Guru Nanak Dev Univ., Amritsar, 143 005, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1996), 35B(5), 409-12

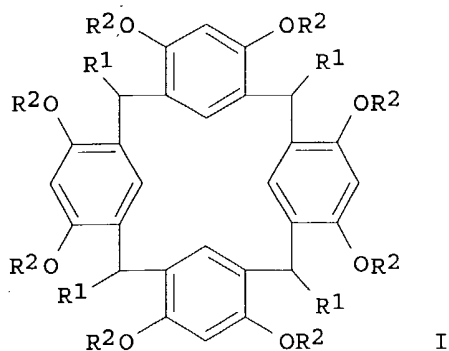
CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: Publications & Information Directorate, CSIR

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



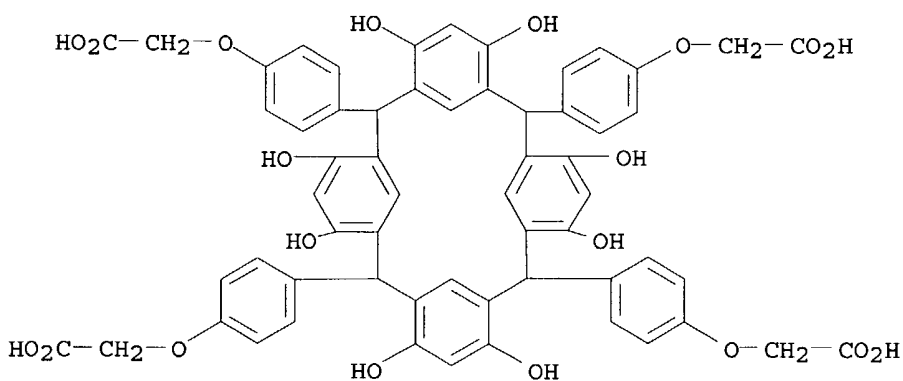
AB Resorcinol-p-hydroxybenzaldehyde tetramer Ia ( $R_1 = p\text{-C}_6\text{H}_4\text{OH}$ ,  $R_2 = \text{H}$ ) has been obtained under acidic conditions, separated into its conformations, and characterized by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra and by the preparation of its octaacetate (Ib;  $R_1 = p\text{-C}_6\text{H}_4\text{OAc}$ ,  $R_2 = \text{H}$ ). The direct carboxymethylation of Ia has been attempted with chloroacetic acid under basic conditions, but due to steric repulsions, tetramer Ic ( $R_1 = p\text{-C}_6\text{H}_4\text{OCH}_2\text{CO}_2\text{H}$ ,  $R_2 = \text{H}$ ) could not be obtained. By use of the reverse approach, p-hydroxybenzaldehyde is carboxymethylated first to yield  $\text{HO}_2\text{CCH}_2\text{O}-p\text{-C}_6\text{H}_4\text{CHO}$  which is then cyclized under acidic conditions to yield the tetramer Id ( $R_1 = p\text{-C}_6\text{H}_4\text{OCH}_2\text{CO}_2\text{Et}$ ,  $R_2 = \text{H}$ ). The coplanar arrangement of carboxylate groups in Ic is utilized to bind uranyl ion. The binding, as shown by a Job's plot, does not show a 1:1 Ic: $\text{UO}_2^{2+}$  ratio due to the fourth carboxylate group, but it acts as a good uranophile as indicated by an increase in the UV absorption intensity of  $\text{UO}_2^{2+}$  ions in the presence of Ic ( $R_1 = p\text{-C}_6\text{H}_4\text{OCH}_2\text{CO}_2\text{Et}$ ,  $R_2 = \text{COCH}_3$ ).

IT 176798-35-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and uranophilic activity of resorcinol-hydroxybenzaldehyde tetramer)

RN 176798-35-9 CAPLUS

CN Acetic acid, 2,2',2'',2'''-[(4,6,10,12,16,18,22,24-octahydropentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-2,8,14,20-tetrayl)tetrakis(4,1-phenyleneoxy)]tetrakis- (9CI) (CA INDEX NAME)



L3 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:994163 CAPLUS

DOCUMENT NUMBER: 124:55584

TITLE: Preparation of calixarene-based compounds having antibacterial, antifungal, anticancer, and anti-HIV activity

INVENTOR(S): Harris, Stephen J.

PATENT ASSIGNEE(S): Ire.

SOURCE: PCT Int. Appl., 148 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9519974	A2	19950727	WO 1995-IE8	19950124
WO 9519974	A3	19950921		
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, FI, GB, HU, JP, KP, LU, NO, RO, UA, US				
RW: AT, BE, CH, DE, ES, FR, GB, GR, IE, LU, NL, SE, GA, ML, NE, SN, TD, TG				
AU 9515453	A1	19950808	AU 1995-15453	19950124
PRIORITY APPLN. INFO.:			IE 1994-57	19940124
			WO 1995-IE8	19950124

THE SOURCE(S) : MARPAT 124:55584

For diagram(s), see printed CA Issue.

B Calixarene-based compds., which are calixarenes or oxacalixarenes, acyclic phenyl-formaldehyde oligomers, cyclotrimeratrylene derivs., cyclic tetrameric resorcinol-aldehyde derivs. known as Hogberg compds. and cyclic tetrameric pyrogallol-aldehyde derivs., are prepared For example, calixarenes or oxacalixarenes are represented by general formula [I;  $n + m = 3-8$ ;  $m = 0-3$ ;  $n = 0-8$ ;  $R_1 = H$ , halo, hydrocarbyl, aryl, (un)substituted hydrocarbylaryl,  $NO_2$ ,  $SO_3M_1$ ; wherein  $M_1 =$  alkali metal,  $SO_3H$ ;  $R_1 = OR_2$ ; wherein  $R_2 = CH_2CO_2R_3$ ,  $CH_2CO_2Mp/p$ ,  $CH_2CONR_4R_5$ ; wherein  $R_3 =$  (un)substituted alkyl;  $M =$  metal, ammonium ion;  $p =$  the charge on the metal ion;  $R_4$  or  $R_5$  may be the same or different, or both may be part of amino acid ester of poly(amino acid ester) or one or more of the same or different amino acids or part of a cyclic polyene antibiotic/antifungal drug or part of a cyclic nitrogen heterocycle;  $X =$  halo,  $NO_2$ ,  $CO_2H$ , cyano, other electron withdrawing group]. Thus, n-butyraldehyde and pyrogallol in a 1:4 mixture of 37% aqueous HCl and EtOH was refluxed under N for 90 min to give a cyclic tetramer (II;  $R = X = H$ ), which was brominated with Br in  $CHCl_3$  to II ( $R = H$ ,  $X = Br$ ) and etherified with Et bromoacetate in the presence of  $K_2CO_3$  in refluxing acetone to give II ( $R = CH_2CO_2Et$ ,  $X = Br$ ). The latter compound was saponified with KOH in refluxing EtOH, acidified with aqueous HCl, and treated with 25% aqueous  $NH_4OH$  to give II ( $R = CH_2CO_2-NH_4^+$ ,  $X = Br$ ). The latter compound in vitro inhibited the infection of C8166 cells with HIV-2, SIV (Simian immunodeficiency virus), and HIV-1 with EC50 of 10, 20, and 0.03  $\mu M$ .

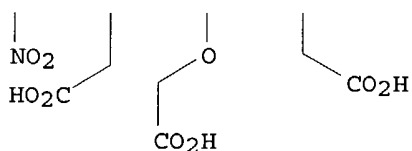
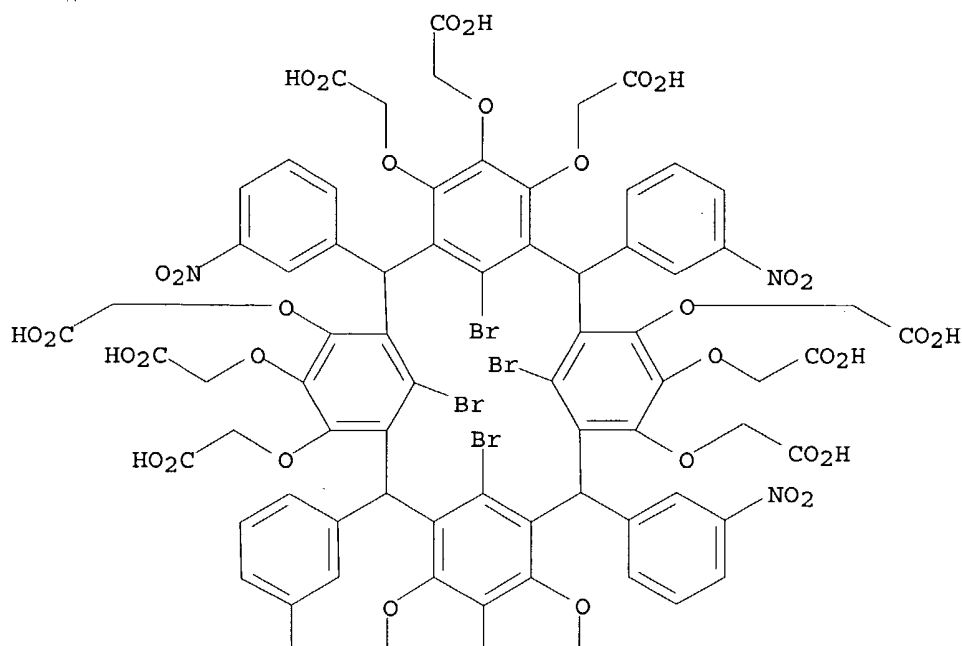
T 171799-65-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of calixarene-based compds. having antibacterial, antifungal, anticancer, and anti-HIV activity)

N 171799-65-8 CAPLUS

N Acetic acid, 2,2',2'',2''',2'''',2''''',2''''',2''''',2''''',2''''',  
 ''',2''''''''',2'''''''''- [[25,26,27,28-tetrabromo-2,8,14,20-tetrakis(3-  
 nitrophenyl)pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-  
 4,5,6,10,11,12,16,17,18,22,23,24-dodecayl]dodecakis(oxy)]dodecakis-,  
 dodecapotassium salt (9CI) (CA INDEX NAME)



● 12 K

ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN  
 CESSION NUMBER: 1995:298047 CAPLUS  
 CUMENT NUMBER: 123:169331  
 TLE: Macrocyclic  $\pi$ -Conjugated Carbopolyanions and  
 Polyradicals Based upon Calix[4]arene and  
 Calix[3]arene Rings  
 THOR(S): Rajca, Andrzej; Rajca, Suchada; Desai, Shailesh R.  
 RPORATE SOURCE: Department of Chemistry, University of Nebraska,  
 Lincoln, NE, 68588-0304, USA  
 URCE: Journal of the American Chemical Society (1995),  
 117(2), 806-16  
 CODEN: JACSAT; ISSN: 0002-7863  
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STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Calix[4]arene- and calix[3]arene-based polyether precursors to  
 polyradicals are synthesized.  $\pi$ -Conjugated carbanions, such as  
 calix[4]arene-based tetraanion and calix[3]arene-based trianion, are  
 prepared and studied using NMR spectroscopy and voltammetry. A 4-fold-sym.



conformer for the tetraanion and two non-interconverting conformers (3-fold- and 2-fold-sym.) for the trianion are found on the NMR time scale. Oxidation of the tetraanion gives the corresponding calix[4]arene-based  $S = 2$  tetraradical. However, ESR spectroscopy suggests that the predominant product from oxidation of calix[3]arene-based trianion is the corresponding triradical dimer. The related calix[3]arene-based  $S = 1$  diradical is found to be monomeric. Addnl. characterization of octaradical I and pentaradical II, which were described in a preliminary communication, is presented.

**167014-10-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and characterization of macrocyclic conjugated carbopolyanions and polyradicals based on calixarene rings)

167014-10-0 CAPLUS

Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 2,8,14,20-tetrakis[4-(1,1-dimethylethyl)phenyl]-2,8,14,20-tetramethoxy- (9CI) (CA INDEX NAME)

